Richtmyer-Meshkov Instability via Direct Simulation Monte-Carlo

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In recent years, there has been increasing interest in the simulation of fluid flows via atomistic methods rather than the more traditional continuum techniques based on the Navier-Stokes equations. Atomistic methods include molecular dynamics (MD), in which Newton's equations of motion for a large number of interacting particles are solved numerically, and direct simulation Monte-Carlo (DSMC), a related technique in which explicit interparticle forces are replaced by stochastically simulated collisions [1]. Examples of such atomistic fluid dynamics simulations include the simulation of Rayleigh-Benard convection by MD [2,3] and the simulation of the Rayleigh-Taylor instability by MD [4] and by DSMC [5].

In this highlight, results are presented from some preliminary simulations of the Richtmyer-Meshkov instability (RMI) using DSMC [6]. The RMI occurs when a shock front passes through the interface between two fluids of differing densities. Any roughness or disturbances initially present on the interface before the passage of the shock grow in magnitude, and the two fluids subsequently mix in a characteristic fashion. The RMI is not a true classical instability, since modes on the interface do not experience an initially exponential growth. However, RMI has many traits in common with certain classical instabilities, particularly the Rayleigh-Taylor instability.

The simulations for which results are presented here were done using a one-processor 2D DSMC code, and each simulation required several days on a single workstation. A shock was induced in the fluid by a piston at one end of the domain. The resulting shock front passed through the denser fluid and crossed the interface into the lighter fluid. In order for turbulent mixing to occur in the RMI, the initial shape of the interface must possess perturbations, and in these simulations the shape of the interface was initially set to be a sine curve of wavelength λ and amplitude $a(0)$.

Figure 1 shows a sequence of snapshots from the evolution of the RMI from a DSMC simulation spanning approximately 7μm in length by 1μm in height. The number of particles present varied over the course of the simulation from approximately 15 to 39 million. The density of the light fluid was
$\rho_l = 0.41$ g/cm^3, and that of the heavy fluid was
$\rho_h = 10\,\rho_l = 4.1$ g/cm^3, for an Atwood number of:

$$A = \frac{\rho_h - \rho_l}{\rho_h + \rho_l} = 0.818$$

The piston velocity was 280 m/s, which created a shock front that moved through the heavy fluid at a velocity of 420 m/s. The initial perturbation amplitude-to-wavelength ratio was relatively large, $a(0)/\lambda = 0.16$. In order for the interface to avoid diffusion and remain sharp, all particles in front of the shock were frozen in position relative to one another. This is equivalent to a temperature of 0 in front of the shock. After passage of the shock, particles were allowed to move freely.

Note the development of the characteristic "mushroom caps" in the mixing zone in Fig. 1, as well as the shear-induced curl-up at the fringes of each structure. This behavior is typical of several fluid instabilities, including the RMI,

Fig. 1. A series of snapshots in the development of the Richtmyer-Meshkov instability as simulated by DSMC. White indicates the heavy fluid, black indicates the light fluid, and the red line indicates the position and profile of the shock front.

Rayleigh-Taylor instability, and Kelvin-Helmholtz instability. Also notice that the two structures present do not remain identical, as they would for a periodically perturbed interface in a typical continuum simulation. Atomistic methods, via the thermal fluctuations they contain and that are physically present at the microscopic scale, provide their own mechanisms for symmetry breaking.

In addition to considering the overall development of the RMI, it is interesting to examine the initial growth of the interface width for times shortly after the passage of the shock front. Using only hydrodynamic considerations, Richtmyer [7] has shown that for small $a(0)$, the velocity at which the amplitude of interfacial perturbations grows is given for small times by:

$$\dot{a}(t) = a(0)\, k\, A\, \Delta v$$

Here $a(t)$ is the amplitude as a function of time, $k = 2\pi / \lambda$ is the wavenumber of the perturbation, and Δv is the change in velocity experienced by the interface as a result of the passage of the shock front. Figure 2 shows a comparison between Richtmyer's prediction and results from a DSMC simulation. This simulation was identical to the one described above, except that the amplitude-to-wavelength ratio was smaller, $a(0)/\lambda = 0.02$.

Note that for small times t, the slope of the $a(t)$ curve from the simulation agrees well with Richtmyer's prediction. This serves as a partial validation of linearized hydrodynamics on the small scales described by these simulations, and fits in well with a previous study performed for the initial growth of the Rayleigh-Taylor instability [8].

For animations and other details of the two simulations described above, see *http://www.lanl.gov/orgs/t/t17/staff/jlb/BarberResearch.html*.

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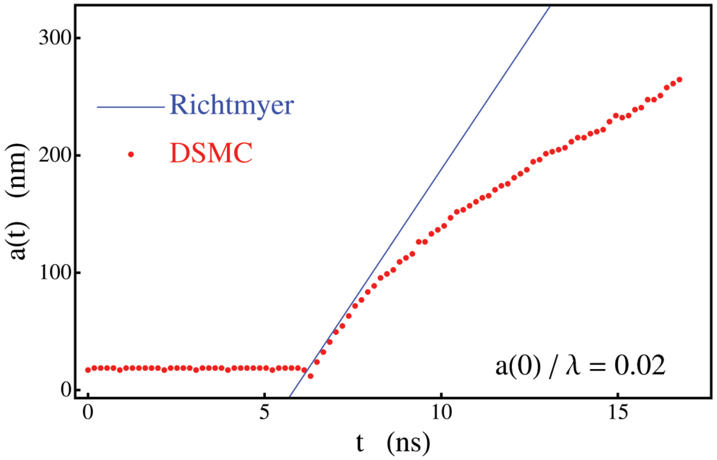

Fig. 2. The amplitude $a(t)$ of an initially sinusoidal perturbation on the interface of the Richtmyer-Meshkov instability as a function of time, as predicted for small t by Richtmyer, and as simulated by DSMC.

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